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Effect of tilt angle on the morphology of SiC epitaxial films grown on vicinal (0001)SiC substrates

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Abstract. In this study of 4H-SiC and 6H-SiC epitaxial films we found that film morphology was strongly dependent on the tilt angle of the substrate. Large surface steps (up to 25 nm high) due to step bunching were more prevalent at smaller tilt angles. Also, 4H films were more susceptible than 6H to 3C-SiC inclusions during growth. The lateral growth of steps from screw dislocations in low-tilt-angle substrates demonstrated that step bunching on the atomic scale was anisotropic with respect to growth direction for both 4H-SiC and 6H-SiC. A model explaining this behavior is presented. We observed and directly measured the Burgers vector of a "super" screw dislocation in a 6H-SiC epilayer.

1. Introduction

Nearly all current SiC epitaxial growth is carried out on vicinal (0001)SiC substrates with the polished growth surface tilted 3° to 5° from the (0001) basal plane[1]. Typical commercial wafers have tilt angles of 3.5°±0.5°[2]. This tilt angle ensures that "step-flow" epitaxial growth occurs (i.e. homoepitaxial growth of the same SiC polytype as the substrate). With regard to epitaxial growth, the tendency for 3C-SiC to nucleate on α-SiC substrates increases as the tilt angle becomes smaller. However, we have shown previously[3] that 6H-SiC can be grown on 6H-SiC at tilt angles as small as 0.1° with proper growth conditions and proper substrate preparation. With regard to morphology, SiC epilayers exhibit a variety of defects and surface features. The dominant features are steps due to macro and atomic-scale step bunching, growth pits, and hillocks[4,5]. This paper presents the results of an investigation of surface morphology of 4H-SiC and 6H-SiC epilayers grown on substrates with tilt angles in the range 0.1° to 3.5°.

2. Experimental

Epilayers of 4H and 6H-SiC were grown by chemical vapor deposition (CVD) by a process reported previously[3]. The SiC substrates were Si-face vicinal (0001) boule- grown wafers obtained from Cree Research[2] with tilt angles ranging from 0.1° to 3.5°. Epilayer thicknesses were typically about 5 μm. The surface morphology of the epilayers was characterized by optical microscopy (OM) and atomic force microscopy (AFM). The AFM (Park Scientific Auto Probe LS) allowed measurement of features down to the atomic scale. The vertical noise level of the AFM was usually less than 0.1 nm which was sufficient to distinguish between atomic step heights that were single or multiples of the unit bilayer SiC step height (0.25 nm) in the c-axis stacking direction . The crystal structure was characterized by transmission electron microscopy (TEM).

3. Results

Macro scale step bunching (steps as high as 25 nm) was observed in some epilayers grown on 3.5°-tilt substrates . Over a given 3.5°-tilt epilayer, the occurrence of large steps was quite variable; large steps were evident over some millimeter-sized regions, but were absent over other millimeter-sized regions. Large steps were always present over the whole area of epilayers with 1.2° and 0.4° tilt angles. An example of large steps on a 0.4° tilt 6H-SiC epilayer is shown in Fig. 1.

Epilayers of 4H were more susceptible than 6H to 3C inclusions. For example, triangular patterns frequently seen[4] in 4H epilayers, but seldom in 6H, were characterized by oxidation[6] and found to contain surface layers of 3C-SiC within some of the triangular areas. Cross section TEM demonstrated the presence of thin planar 3C sections parallel to the (0001) plane in 4H epilayers containing a high density of the triangles. Also, we attempted to grow homoepitaxial films of 4H and 6H on 0.4° tilt 4H and 6H substrates, respectively, in the same growth runs. In every case, no continuous films of 4H were achieved, only 3C films with a high density of double positioning boundaries (DPB's)[3] and isolated 4H hillocks were obtained. In contrast, continuous 6H films on 6H substrates were achieved in most cases.

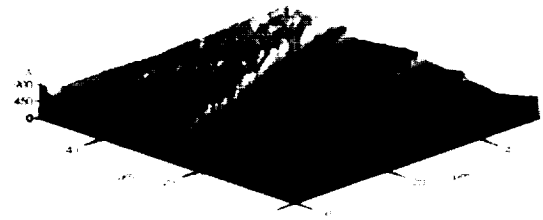

Fig. 1. AFM image of macro step bunching on the surface of a 6H-SiC epilayer with a tilt angle of 0.4°.

Isolated hexagonal hillocks were observed in both 4H and 6H epilayers grown on substrates with tilt angles less than 0.5°. Step bunching on hillocks was quite different from the typical behavior shown in Fig. 1. Multiple spiral patterns of growth steps, assumed to be caused by screw dislocations, propagated from the peak of each hillock. An example is illustrated in Fig. 2, which shows two spirals of 0.5 nm high steps propagating from the peak of a hillock grown on a 4H substrate. Each 0.5 nm step is a doublet step of the basic 0.25 nm high SiC bilayer step. The spiral evolves into a hexagonal pattern as shown. Since the total height of the two steps is 2 x 0.5 = 1.0 nm, the repeat height (Burgers vector) for this screw dislocation is equal to the repeat height of the 4H polytype. Thus, each 0.5 nm step is one of the two doublet steps of the 4H stacking sequence. As can be seen from Fig. 2, the doublet steps bunch to form a wide step, narrow step combination step with a height of 1.0 nm in the $\langle 1\,\bar{1}\,00\rangle$ directions (e.g. $[10\,\bar{1}\,0]$ and $[01\,\bar{1}\,0]$). As the growth direction rotates to the next $\langle 1\,\bar{1}\,00\rangle$ direction, the step pattern undergoes a transition at the $[11\,\bar{2}\,0]$ direction. At this transition direction, the step heights revert back to a doublet step height, i.e. 0.5 nm.

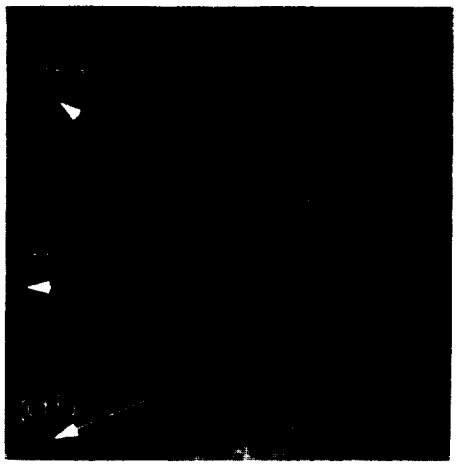

Fig. 2. AFM image of spiral steps propagating from the peak of a 4H-SiC hillock.

An unusual hillock grown on a 6H substrate is shown in Fig. 3. This hillock consists of 16 growth steps propagating from the center of the spiral. The number 16 was determined by following a specific step around one complete revolution and counting the number of steps along the transition region back to the starting point. Each of these 16 steps is a triplet step, 3 x 0.25 nm = 0.75 nm high. These triplet steps bunch into 8 triplet-step pairs in the $\langle 1\,\bar{1}\,00\rangle$ directions. The bunching forms single large steps rather than wide step, narrow step combination steps as was observed for 4H.

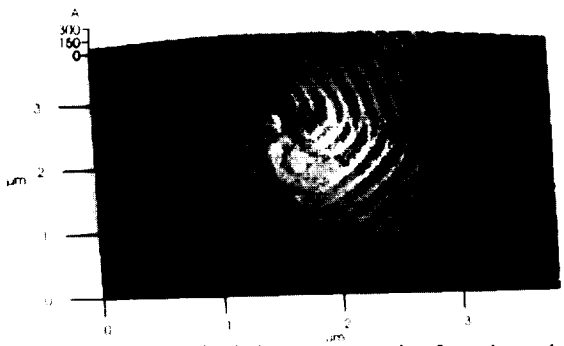

Fig. 3. AFM image of spiral steps propagating from the peak of a 6H-SiC hillock. Steps are produced by a super screw dislocation.

Each triplet-step pair has a total height of 2 x 0.75 nm = 1.5 nm, the repeat height of the 6H polytype. The Burgers vector for this screw dislocation is equal to 8 x the repeat height of the 6H polytype (total height: 12 nm). Screw dislocations with such large Burgers vectors have been called super screw dislocations[7]. The step bunching seen for this hillock is similar to that for the 4H hillock of Fig. 2 except that triplet-step pairs form in the $\langle 1\,\bar{1}\,00\rangle$ directions, instead of doublet-step pairs as was observed for 4H.

4. Discussion

In order to appreciate the significance of the hillock observations, a few aspects of SiC polytypism must be recalled. The 6H structure consists of the stacking of alternate triplet-step layers of the 3C polytype and these are usually designated as ABC and ACB. The difference in structure between these two triplet-step layers is a rotation of 60° about the stacking axis (the c-axis). Similarly, the 4H structure consists of alternate doublet-step layers of the 3C polytype and are designated AB and AC. Sakamoto et al.[8] pointed out that for steps on a Si(111) surface, there are either two dangling bonds per atom or one dangling bond per atom on the step riser depending on the crystallographic direction of the step. Because of threefold symmetry of Si(111), the number of bonds per atom alternates every 60° between one and two as the direction rotates about the surface normal. They suggested that faces (steps) with two dangling bonds per atom grow faster than faces with one dangling bond per atom. We apply these ideas to SiC with the following result. For a given $\{1\,\bar{1}\,00\}$ face of 6H-SiC, there is a particular pattern of one and two dangling bonds per atom; if we assume, for example, that the ABC triplet-step layers in a stacking sequence have one dangling bond per atom on this given $\{1\,\bar{1}\,00\}$ face, then the other triplet-step layers in the sequence (the ACB layers) on this same $\{1\,\bar{1}\,00\}$ face will have two dangling bonds per atom. If one examines the pattern of bonds per atom on adjacent $\{1\,\bar{1}\,00\}$ faces, the pattern is reversed: the ABC triplet-step layers have two bonds per atom, and the ACB triplet-step layers have one bond per atom.

We propose the following model, based on ideas of the previous paragraph, to explain the anisotropic step bunching demonstrated in Figs. 2 and 3. We will use the 4H hillock depicted in Fig. 2 to describe the model. If, in the case of Fig. 2, we designate the top (wider) doublet steps in the $[10\,\bar{1}\,0]$ direction as AB doublet steps and assume that AB steps have two dangling bonds per atom, they will grow faster in this direction than the AC doublet steps which have only one dangling bond per atom; hence, step bunching of doublet-step pairs will occur as shown. If we examine growth in the adjacent $\langle 1\,\bar{1}\,00\rangle$direction (e.g. the $[01\,\bar{1}\,0]$ direction) the AB steps will now be growing slower because they will have only one dangling bond per atom, and the AC steps will now be growing faster; hence reversed step bunching will occur. In this new direction (i.e.$[01\,\bar{1}\,0]$), the faster growing AC steps becomes the top (wider) step , overtaking the slower growing AB steps. The transition between these two states causes a localized "debunching" of the paired doublet steps in the $[11\,\bar{2}\,0]$ direction between the two adjacent $\langle 1\,\bar{1}\,00\rangle$ directions. The same process occurs for 6H-SiC triplet steps as shown in Fig. 3.

Calculations were recently carried out by Heuell et al.[9] on the lateral growth of steps on a 6H-SiC vicinal (0001) surface tilted in a $\langle 1\,\bar{1}\,00\rangle$ direction. They assumed (1) single bilayer steps on the surface and (2) each successive group of steps consists of one dangling bond per atom on the leading step edge of three successive steps followed by two bonds per

atom on the next successive three steps. The result of the calculations indicated that the single bilayer steps structure would evolve into a structure with a step height of six bilayers. Our results are consistent with these calculations. Also, our model explains the occurrence of 0.75 nm height steps when 1.5 nm high steps turn by 60° as observed by Tyc[10] on a sublimation-grown epilayer on a 6H-SiC Lely crystal.

As can be seen in Figs. 2 and 3, the transition between the two bunched-step orientations in adjacent $\langle 1\,\bar{1}\,00\rangle$ directions occurs over a very small angular change in growth direction in the vicinity of the $\langle 11\,\bar{2}\,0\rangle$ direction between these two $\langle 1\,\bar{1}\,00\rangle$ directions. The instability in step bunching in this transition region may be a factor in the macro scale step bunching that is observed in the SiC epilayers. Any small undulation of the growth surface, or defect on the surface could aggravate the effect of this instability. This may be significant since most SiC epilayer growth is carried out on vicinal (0001) wafers tilted toward a $\langle 11\,\bar{2}\,0\rangle$ direction.

Previously, we have found that dislocations and micropipes propagate from the SiC substrate into the epilayer[11]. Hence, we believe that all of the observed hillocks are produced from screw dislocations that have their origin in the substrate. The observation and direct measurement of the Burgers vector of the super screw dislocation illustrated in Fig. 3 is significant because it is believed that the formation of micropipes[12] is associated with strain caused by the presence of super screw dislocations[13].

5. Conclusions

This investigation of epitaxial growth on SiC substrates with small tilt angles has yielded significant new information on SiC crystal growth processes. For example, under the conditions used in our CVD process, the 4H polytype is more susceptible than 6H to 3C inclusions, and this tendency became worse at smaller tilt angles. Also, the tendency for macro step bunching was shown to be greater at smaller tilt angles. The investigation of hillocks that are produced on substrates with small tilt angles led to the demonstration of anisotropic atomic scale step bunching in 4H and 6H epilayer growth. The anisotropic behavior is consistent with a model we proposed that is based on the anisotropic distribution of the number of dangling bonds per atom in the various $\langle 1\,\bar{1}\,00\rangle$ directions.

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